

FROM LOW-RANK APPROXIMATION TO AN EFFICIENT RATIONAL KRYLOV SUBSPACE METHOD FOR THE LYAPUNOV EQUATION

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Abstract. We propose a new method for the approximate solution of the Lyapunov equation with rank-1 right-hand side, which is based on extended rational Krylov subspace approximation with adaptively computed shifts. The shift selection is obtained from the connection between the Lyapunov equation, solution of systems of linear ODEs and alternating least squares method for low-rank approximation. The numerical experiments confirm the effectiveness of our approach.

Key words. Lyapunov equation, rational Krylov subspace, low-rank approximation, model order reduction

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1. Introduction. Let A be an $n \times n$ stable matrix and y_0 is a vector of length N . We consider the continuous-time Lyapunov equation with rank-1 right-hand side:

$$AX + XA^\top = -y_0 y_0^\top, \quad (1.1)$$

For large n it is impossible to store X , thus a low-rank approximation of the solution is sought:

$$X \approx UZU^\top, \quad U \in \mathbb{R}^{n \times r}, \quad Z \in \mathbb{R}^{r \times r}. \quad (1.2)$$

Lyapunov equation has fundamental role in many application areas such as signal processing [15, 31] and system and control theory [5, 22, 27]. There are many approaches for the solution of the Lyapunov equation. Alternating directions implicit (ADI) methods [21, 24, 23, 18] are powerful techniques that arise from the solution methods for elliptic and parabolic partial differential equations [39, 6, 4, 16].

Krylov subspace methods have been successful in solving linear systems and eigenvalues problems. They utilize Arnoldi-type [19, 36, 17] or Lanczos-type [29, 1] algorithms to construct low-rank approximation using Krylov subspaces. Krylov subspace methods have advantage in simplicity but the convergence can be slow for ill-conditioned A [34, 25].

Rational Krylov subspace methods (extended Krylov subspace method [7, 32], adaptive rational Krylov [34, 8, 9, 10], Smith method [14, 26]) are often the method of choice. Manifold-based approaches have been proposed in [38, 37] where the solution is sought directly in the low-rank format (1.2). The main computational cost in such algorithms is the solution of linear systems with matrices of the form $A + \lambda_i I$. A comprehensive review on the solution of linear matrix equations in general and Lyapunov equation in particular can be found in [33].

In this work we start from the Lyapunov equation and a simple method that doubles the size of U at each step using the solution of an auxiliary Sylvester equation. The main disadvantage of this approach is that too many linear system solvers are required for each step. Using the rank-1 approximation to the correction equation,

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we obtain a simple formula for the new vector. In our experiments we also found that it is a good idea to add a Krylov vector to the subspace. This increases the accuracy significantly at almost no additional cost. We compare the effectiveness of the new method with the extended rational Krylov method [7, 32] and the adaptive rational Krylov approach [8, 9] on several model examples with symmetric and non-symmetric matrices A coming from discretizations of two-dimensional and three-dimensional elliptic PDEs on different grids.

2. Minimization problem. How do we define what is the best low-rank approximation to the Lyapunov equation? A natural way is to formulate the initial problem as a minimization problem

$$R(X) \rightarrow \min,$$

and then reduce this problem to the minimization over the manifold of low-rank matrices. A popular choice is the residual:

$$R(X) = \|AX + XA^\top + y_0 y_0^\top\|_F^2, \quad (2.1)$$

which is easy to compute for a low-rank matrix X . Disadvantage of the functional (2.1) is well known: it may lead to the large condition numbers [20, p. 19]. For the symmetric positive definite case another functional is often used:

$$R(X) = \text{tr}(XAX) + \text{tr}(Xy_0 y_0^\top).$$

For a non-symmetric case we can use a different functional, which is based on the connection of the low-rank solution to the Lyapunov equation and low-dimensional subspace approximation to the solution of a system of linear ODEs. Consider an ODE with the matrix A :

$$\frac{dy}{dt} = Ay, \quad y(0) = y_0.$$

It is natural to look for the solution in the low-dimensional subspace form

$$y(t) \approx \tilde{y}(t) = Uc(t),$$

where U is an $n \times r$ orthogonal matrix and $c(t)$ is an $r \times 1$ vector. Then the columns of the orthogonal matrix U that minimizes

$$\begin{aligned} & \min_{U \in O(n), c(t)} \int_0^\infty \|y(t) - \tilde{y}(t)\|^2 dt = \\ &= \min_{U \in O(n)} \int_0^\infty \|y(t) - UU^\top y(t)\|^2 dt + \min_{U \in O(n), c(t)} \int_0^\infty \|UU^\top y(t) - \tilde{y}(t)\|^2 dt = \\ &= \min_{U \in O(n)} \int_0^\infty \|y(t) - UU^\top y(t)\|^2 dt = \min_{U \in O(n)} \left(\text{tr } X - \text{tr } U^\top XU \right) \end{aligned}$$

are the eigenvectors, corresponding to the largest eigenvalues of the matrix X [35] that solves the Lyapunov equation (1.1). However, the computation of the optimal

$\widehat{c}(t) = U^\top y(t)$ requires the knowledge of the true solution $y(t)$ which is not known. Instead, we can consider the Galerkin projection:

$$\begin{aligned}\widetilde{y} &= Uc(t), \\ \frac{dc}{dt} &= U^\top AUc, \quad c_0 = U^\top y_0,\end{aligned}\tag{2.2}$$

The final approximation is then

$$\widetilde{y} = Ue^{Bt}U^\top y_0,\tag{2.3}$$

where $B = U^\top AU$. The functional to be minimized is

$$F(U) = \int_0^\infty \|y - \widetilde{y}\|^2 dt.\tag{2.4}$$

Note that the functional depends only on U . Given U , the approximation to the solution of the Lyapunov equation can be recovered from the solution of the “small” Lyapunov equation

$$X \approx UZU^\top, \quad BZ + ZB^\top = -c_0c_0^\top.\tag{2.5}$$

The functional (2.4) can not be efficiently computed. However, a simple expansion of the norm gives

$$F(U) = \int_0^\infty \|y\|^2 dt - 2 \int_0^\infty \langle y, \widetilde{y} \rangle dt + \int_0^\infty \|\widetilde{y}\|^2 dt.\tag{2.6}$$

Let us represent the functional in the next form

$$F(U) = F_1(U) - 2F_2(U),$$

where

$$F_1(U) = \int_0^\infty (\|y\|^2 - \|\widetilde{y}\|^2) dt, \quad F_2(U) = \int_0^\infty (\langle y, \widetilde{y} \rangle - \|\widetilde{y}\|^2) dt.$$

LEMMA 2.1. *Assume that matrices A and B are stable. Then the functionals $F_1(U), F_2(U)$ can be calculated as follows:*

$$\begin{aligned}F_1(U) &= \text{tr } X - \text{tr } Z, \\ F_2(U) &= \text{tr } U^\top (P - UZ),\end{aligned}\tag{2.7}$$

where P is the solution of the Sylvester equation and Z is solution of the Lyapunov equation:

$$\begin{aligned}AP + PB^\top &= -y_0c_0^\top, \\ BZ + ZB^\top &= -c_0c_0^\top.\end{aligned}\tag{2.8}$$

Proof:

It is easy to see, that

$$\begin{aligned} -\int_0^\infty \langle y, \tilde{y} \rangle dt &= -\text{tr} \int_0^\infty e^{At} y_0 c_0^\top e^{B^\top t} U^\top dt = -\text{tr} \left(e^{At} P e^{B^\top t} U^\top \right) \Big|_0^\infty = \text{tr} U^\top P, \\ \int_0^\infty \|\tilde{y}\|^2 dt &= \text{tr} \int_0^\infty U e^{Bt} c_0 c_0^\top e^{B^\top t} U^\top dt = -\text{tr} \left(e^{Bt} Z e^{B^\top t} \right) \Big|_0^\infty = \text{tr} Z. \end{aligned}$$

In the same way $\int_0^\infty \|y\|^2 dt = \text{tr} X$ and we can write

$$\begin{aligned} F_1(U) &= \int_0^\infty \left(\|y\|^2 - \|\tilde{y}\|^2 \right) dt = \text{tr} X - \text{tr} Z, \\ F_2(U) &= \int_0^\infty \left(\langle y, \tilde{y} \rangle - \|\tilde{y}\|^2 \right) dt = \text{tr}(U^\top P - Z) = \text{tr} U^\top (P - UZ). \blacksquare \end{aligned}$$

Note that using integral representation of the solution of Lyapunov equation is well-known fact [28]:

$$X = -\int_0^\infty e^{At} y_0 y_0^\top e^{A^\top t} dt.$$

The Sylvester equation can be solved using a standard method [35, Theorem 3.1] since the matrix B is $r \times r$, $r \ll n$. We compute the Schur decomposition of B^\top and the equation is reduced to r linear systems with the matrices $A + \lambda_i I$, $i = 1, \dots, r$.

LEMMA 2.2. *Assume that matrices A and B are stable. The gradient of $F(U)$ can be computed as:*

$$\begin{aligned} \text{grad} F(U) &= -2P + 2y_0(c_0^\top Z_I - y_0^\top P_U) + 2AU(ZZ_I - P^\top P_U) + \\ &\quad + 2A^\top U(Z_I Z - P_U^\top P), \end{aligned} \tag{2.9}$$

where P, Z are defined by (2.8) and

$$\begin{aligned} A^\top P_U + P_U B &= -U, \\ B^\top Z_I + Z_I B &= -I_r. \end{aligned} \tag{2.10}$$

Proof:

Variation of Z can be expressed as a solution of the Lyapunov equation with another right hand side:

$$B\delta Z + \delta Z B^\top = -\delta c_0 c_0^\top - c_0 \delta c_0^\top - \delta B Z - Z \delta B^\top$$

Using the well-known integral form of the solution of the Lyapunov equation we get that:

$$\begin{aligned}
-\operatorname{tr} \delta Z &= -\operatorname{tr} \int_0^\infty e^{Bt} (\delta c_0 c_0^\top + c_0 \delta c_0^\top + \delta B Z + Z \delta B^\top) e^{B^\top t} dt = \\
&= -\operatorname{tr} \left(\int_0^\infty e^{B^\top t} I e^{Bt} dt \right) (\delta c_0 c_0^\top + c_0 \delta c_0^\top + \delta B Z + Z \delta B^\top) = \\
&= -\operatorname{tr} Z_I (\delta c_0 c_0^\top + c_0 \delta c_0^\top + \delta B Z + Z \delta B^\top) = \\
&= -2 \operatorname{tr} \delta U^\top (y_0 c_0^\top Z_I + A U Z Z_I + A^\top U Z_I Z).
\end{aligned}$$

Similarly for P :

$$A \delta P + \delta P B^\top = -y_0 \delta c_0^\top - P \delta B^\top,$$

therefore,

$$\begin{aligned}
\delta \operatorname{tr}(U^\top P) &= \operatorname{tr}(\delta U^\top P + U^\top \delta P) = \\
&= \operatorname{tr}(\delta U^\top P + U^\top \int_0^\infty e^{At} (y_0 \delta c_0^\top + P \delta B^\top) e^{B^\top t} dt) = \\
&= \operatorname{tr} \delta U^\top P + \operatorname{tr} \left(\int_0^\infty e^{B^\top t} U^\top e^{At} dt \right) (y_0 \delta c_0^\top + P \delta B^\top) = \\
&= \operatorname{tr} \delta U^\top P + \operatorname{tr} P_U^\top (y_0 \delta c_0^\top + P \delta B^\top) = \\
&= \operatorname{tr} \delta U^\top (P + y_0 y_0^\top P_U + A^\top U P_U^\top X + A U P^\top P_U).
\end{aligned}$$

Finally,

$$\begin{aligned}
\delta F(U) &= \operatorname{tr} \delta U^\top (\operatorname{grad} F) = \operatorname{tr} \delta (-2U^\top P + Z), \\
\operatorname{grad} F(U) &= -2P + 2y_0(c_0^\top Z_I - y_0^\top P_U) + 2AU(ZZ_I - P^\top P_U) + \\
&\quad + 2A^\top U(Z_I Z - P_U^\top P). \blacksquare
\end{aligned}$$

Now denote by $R_1(U)$ and $R_2(U)$ residuals of the Lyapunov and Sylvester equations:

$$\begin{aligned}
R_1(U) &= \|A(UZU^\top) + (UZU^\top)A^\top + y_0 y_0^\top\|, \\
R_2(U) &= \|A(UZ) + (UZ)B^\top + y_0 c_0^\top\|.
\end{aligned} \tag{2.11}$$

LEMMA 2.3. Assume that matrices A and B are stable and y_0 lies in the column space of U . Then the next equality holds:

$$R_1(U) = \sqrt{2} R_2(U) = \sqrt{2} \|(AU - UB)Z\|. \tag{2.12}$$

Proof:

Since Z is the unique solution of the Lyapunov equation, we get that

$$\begin{aligned}
R_1(U)^2 &= \|AUZU^\top + UZU^\top A^\top + y_0 y_0^\top\|^2 = \\
&= \|y_0 y_0^\top - UU^\top y_0 y_0^\top UU^\top + (AU - UB)ZU^\top + UZ(AU - UB)^\top\|^2 = \\
&= \|(AU - UB)ZU^\top\|^2 + \|UZ(AU - UB)^\top\|^2 = 2\|(AU - UB)Z\|^2.
\end{aligned}$$

We can use the same trick for the residual of the Sylvester equation:

$$\begin{aligned}
R_2(U)^2 &= \|A(UZ) + (UZ)B^\top + y_0 c_0^\top\|^2 = \\
&= \|(I - UU^\top)y_0 c_0^\top + (AU - UB)Z\|^2 = \|(AU - UB)Z\|^2. \blacksquare
\end{aligned}$$

Lemma 2.3 is well known for the special case when U is the basis of a (rational) Krylov subspace [17, Theorem 2.1]. Lemma 2.3 is valid if $y_0 \in \text{span } U$ and we will always make sure that $y_0 = UU^\top y_0$. The next Lemma shows that if the residual of the Lyapunov equation goes to zero, so does the values of the functional $F(U)$.

LEMMA 2.4. *Assume that matrices A and B are stable and y_0 lies in the column space of U . Then*

$$F(U) \leq CR_1(U)$$

with a constant

$$C = \left\| \left(I \otimes A + A \otimes I \right)^{-1} \right\|_F + \sqrt{2r} \left\| \left(I \otimes A + B \otimes I \right)^{-1} \right\|_F.$$

Proof:

The matrix $X - UZU^\top$ satisfies the Lyapunov equation

$$A(X - UZU^\top) + (X - UZU^\top)A^\top = -(AU - UB)ZU^\top - UZ(AU - UB)^\top,$$

therefore

$$(I \otimes A + A \otimes I) \text{vec} \left(X - UZU^\top \right) = -\text{vec} \left((AU - UB)ZU^\top + UZ(AU - UB)^\top \right),$$

and

$$\|X - UZU^\top\|_F \leq \left\| \left(I \otimes A + A \otimes I \right)^{-1} \right\|_F R_1(U)$$

Thus,

$$|\text{tr } X - \text{tr } Z| \leq C_1 R_1(U).$$

In the same way,

$$\|P - UZ\|_F \leq \left\| \left(I \otimes A + B \otimes I \right)^{-1} \right\|_F R_2(U) = C_2 R_2(U),$$

therefore

$$|F_2(U)| = |\text{tr } U^\top (P - UZ)| \leq \|U\|_F \|P - UZ\|_F \leq \sqrt{r} C_2 R_2(U).$$

Finally,

$$F(U) \leq |F_1(U)| + 2|F_2(U)| \leq (C_1 + \sqrt{2r} C_2) R_1(U) = CR_1(U).$$

■

Lemma 2.4 shows that $R_1(U)$, the residual of the Lyapunov equation, is a viable error bound for our functional $F(U)$.

LEMMA 2.5. *Assume that matrices A and B are stable, y_0 lies in the column space of U , matrices P and Z are solutions of the Sylvester and the small Lyapunov equations 2.8 correspondingly. Then*

$$\|X - PU^\top - UP^\top + UZU^\top\|_F \leq F(U).$$

Proof:

Let us consider the matrix

$$M = \int_0^\infty (y(t) - \tilde{y}(t)) (y^\top(t) - \tilde{y}^\top(t)) dt.$$

We use exponential representations of the Lyapunov and the Sylvester equations solutions (2.8):

$$\begin{aligned} M &= \int_0^\infty y(t) y^\top(t) dt - \int_0^\infty \tilde{y}(t) y^\top(t) dt - \int_0^\infty y(t) \tilde{y}^\top(t) dt + \int_0^\infty \tilde{y}(t) \tilde{y}^\top(t) dt = \\ &= X - PU^\top - UP^\top + UZU^\top. \end{aligned}$$

Matrix M is symmetric and non-negative definite and therefore:

$$\|X - PU^\top - UP^\top + UZU^\top\|_F = \|M\|_F \leq \text{tr } M = F(U) \quad (2.13)$$

■

We can also compare $F(U)$ functional based on Galerkin projection with functional based on optimal projection $\hat{y} = UU^\top y(t)$:

$$\begin{aligned} \int_0^\infty \|y(t) - \hat{y}(t)\|^2 dt &= \text{tr}(I - UU^\top)X(I - UU^\top) = \\ &= \text{tr}(I - UU^\top)M(I - UU^\top) \leq \text{tr } M = F(U). \end{aligned} \quad (2.14)$$

Lemma 2.5 shows that if $F(U)$ is small, the solution X can be well-approximated by a rank- $2r$ matrix.

3. Methods for basis enrichment. Notice that the column vectors of the gradient are a linear combination of the column vectors of $P, AU, A^\top U$ and y_0 . We need a method to enlarge the basis U so the first idea is to use matrix P to extend the basis. Note, that the matrix UZ can be also considered as an approximation to the solution of Sylvester equation. So to enrich the basis we will use $P_1 = P - UZ$ instead, and the matrix P_1 satisfies the equation:

$$\begin{aligned} A(P - UZ) + (P - UZ)B^\top &= -y_0 c_0^\top - AUZ - UZB^\top = \\ &= -(I - UU^\top)y_0 c_0^\top - (AU - UB)Z, \\ AP_1 + P_1 B^\top &= -(AU - UB)Z, \end{aligned} \quad (3.1)$$

where we have used that $y_0 = UU^\top y_0$.

The method is summarized in Algorithm 1. The main disadvantage of Algorithm 1 is that the computational cost grows dramatically at each step. If U has r columns, the next step will require r solutions of $n \times n$ linear systems with matrices of the form

$A + \lambda_i I$.

Algorithm 1: The doubling method

Data: Input matrix $A \in \mathbb{R}^{n \times n}$, vector $y_0 \in \mathbb{R}^{n \times 1}$, maximal rank r_{\max} , accuracy parameter ε .

Result: Orthonormal matrix $U \in \mathbb{R}^{n \times r}$.

begin

- 1 set $U = \frac{y_0}{\|y_0\|}$ ▷ Initialization
- 2 **for** rank $U \leq r_{\max}$ **do**
- 3 Compute $c_0 = U^\top y_0$, $B = U^\top A U$
- 4 Compute Z as Lyapunov equation solution: $BZ + ZB^\top = -c_0 c_0^\top$
- 5 Compute error estimate $\delta = \|(AU - UB)Z\|$
- 6 **if** $\delta \leq \varepsilon$ **then**
- 7 Stop
- 8 Compute P_1 as Sylvester equation solution:
 $AP_1 + P_1 B^\top = -(AU - UB)Z$
- 9 Update $U = \text{orth}[U, P_1]$

REMARK 3.1. *Algorithm 1 is similar to the IRKA method [2, 12, 13, 11]. The IRKA method starts from initial orthogonal matrices V_0, W_0 with the given rank r and replaces the matrices V_{i-1} and W_{i-1} by the new ones V_i and W_i that are the union of the rational Krylov subspaces $(A + s_i I)^{-1}b$ and $(A^\top + s_i I)^{-1}c$, correspondingly, in every step. The shifts s_i are obtained as eigenvalues of the matrix $V_{i-1}^\top A W_{i-1}$. The main difference of Algorithm 1 algorithm from IRKA is that IRKA is usually used with the fixed rank.*

To reduce the number of solvers required by the algorithm, we propose two improvements. The first is to add the last Krylov vector to the subspace. In this case, as we will show, the residual will always have rank-1. The second improvement is to add only one vector each time. In order to do so, we will use a simple rank-1 approximation to P_1 .

3.1. Adding a Krylov vector and a rational Krylov vector to the subspace. In the following section we will show, that under a special basis enrichment strategy, the rank-1 approximation to P_1 can be replaced by adding one vector of the form $(A + sI)^{-1}w$ to the subspace. In this case, as it was already described in [32, 34], adding a Krylov vector preserves the rank-1 structure of the residual of equation (3.1). Next Lemma is a generalization of the well-known fact of rank-1 residual in the Arnoldi iteration [30].

LEMMA 3.1. *Let A be an $n \times n$ stable matrix and y_0 is a vector of size n . Assume that an $n \times r$ orthogonal matrix U and vectors w, v of size n satisfy the following equations:*

$$(I - UU^\top)AU = wq^\top, \quad v = (A + sI)^{-1}w.$$

Let us denote by U_1 and U_2 the basis of the spans of the columns of the matrices $[U, v]$ and $[U, v, w]$ accordingly. Then the following equality holds

$$(I - U_2 U_2^\top)AU_2 = (I - U_2 U_2^\top)Aw\hat{q}^\top.$$

Proof:

Due to the fact that $(I - UU^\top)AU = wq^\top$ we get that $(I - U_2 U_2^\top)AU = 0$.

On the other hand we have

$$(I - U_2 U_2^\top)Av = (I - U_2 U_2^\top)((A + sI)v - sv) = (I - U_2 U_2^\top)(w - sv) = 0.$$

Therefore $(I - U_2 U_2^\top)AU_2 = (I - U_2 U_2^\top)Awq^\top$. Note that if U_1 and U_2 are obtained by using the Gram-Schmidt process then $(I - U_2 U_2^\top)AU_1 = 0$ and the matrix $(I - U_2 U_2^\top)AU_2$ has only one non-zero column and this column is the last one. ■

The statements about residual rank-structure are well known [17, 32]. Lemma 3.1 shows that if the approximation algorithm starts from $U_0 = \frac{y_0}{\|y_0\|}$ and adds a vector from the Krylov subspace and a corresponding vector from the rational Krylov subspace at each step then the residual matrix $(AU - UB)Z = (I - UU^\top)AUZ$ is rank-1 at any step. That is the main benefit from using the Krylov subspaces in our approach. Moreover, the residual has the form $\hat{w}\hat{q}^\top$, where $\hat{w} = (I - U_1 U_1^\top)Aw$ is the next *Krylov vector*. This fact is important and will be used later.

3.2. Rank-1 approximation to the correction equation. Suppose we have the matrix U constructed by sequential addition of rational Krylov and Krylov vectors to the subspace and the equation for P_1 has the form (3.1) Note, that due to the equality

$$(AU - UB) = (I - UU^\top)AU,$$

the matrix $(AU - UB) = wq^\top$ has only one non-zero column. If the new vectors are added as the rightmost vectors,

$$(AU - UB)Z = wz^\top,$$

where z^\top is the last row of the matrix Z . Therefore, the equation for P_1 takes the form

$$AP_1 + P_1 B^\top = -(AU - UB)Z = wz^\top. \quad (3.2)$$

The last step from the doubling method to the final algorithm is find to a rank-1 approximation to the solution of (3.2). If U is known, we apply one step of alternating iterations, looking for the solution in the form $P_1 \approx vq^\top$, where $q = \frac{z}{\|z\|}$ is the normalized last row of the matrix Z . This choice of q is natural due to the right hand side of (3.2): $-(AU - UB)Z = \|z\|wq^\top$. The Galerkin condition for v leads to equation

$$(A + (q^\top B^\top q) I) v = w.$$

This is the main formula for the next shift. Due to the simple rank-1 structure of the residual its norm can be efficiently computed as

$$R_1(U) = \sqrt{2}\|w\| \|z\|.$$

The final algorithm which we call *alternating low rank (ALR) method* is presented in Algorithm 2. The main computational cost is the solution of the shifted linear system.

Algorithm 2: The Adaptive low-rank method

Data: Input matrix $A \in \mathbb{R}^{n \times n}$, vector $y_0 \in \mathbb{R}^{n \times 1}$, maximal rank r_{\max} , accuracy parameter ε .

Result: Orthonormal matrix $U \in \mathbb{R}^{n \times r}$.

begin

```

1  set  $U = \frac{y_0}{\|y_0\|}, w_0 = \frac{y_0}{\|y_0\|}$  ▷ Initialization
2  for rank  $U \leq r_{\max}$  do
3      Compute  $w_k = (I_n - UU^\top)Aw_{k-1}$ 
4      Compute  $c_0 = U^\top y_0, \quad B = U^\top AU$ 
5      Compute  $Z$  as Lyapunov equation solution:  $BZ + ZB^\top = -c_0 c_0^\top$ 
6      Compute  $z$  as the last row of the matrix  $Z$ .
7      Compute error estimate  $\delta = \|w_k\| \|z\|$ 
8      if  $\delta \leq \varepsilon$  then
9           $\hookrightarrow$  Stop
10     Compute shift  $s = q^\top Bq, q = \frac{z}{\|z\|}$ 
11     Compute  $v_k = (A + sI)^{-1}w_k$ 
12     Update  $U := \text{orth}[U, v_k, w_k]$ .
```

Remark. Restriction to rank-1 right hand sides is helpful because there are several ways to generalize ALR algorithm for an arbitrary rank case. We can either go for rank-1 approximation to the solution of the Sylvester equation (and get one new Rational Krylov vector each time), or use a block version of the ALR algorithm. We plan to compare this approaches in our future work.

4. Numerical experiments. We have implemented the ALR method in Python using SciPy and NumPy packages available in the Anaconda Python distribution. The implementation is available online at https://github.com/dkolesnikov/rkm_lyap. The matrices, Python code and IPython notebooks which reproduce all the figures in this work are available at <https://github.com/dkolesnikov/alr-paper>, where the .mat files with test matrices and vectors can be found as well. We have compared the ALR method with two methods with publicly available Matlab implementations. We have ported all the methods to Python for a fair comparison, and their implementations are also online.

The first method uses the Extended Krylov Subspaces approach which was proposed in [7]. Its main idea is to use as the basis the *extended Krylov subspace* of the form

$$\text{span} \left(A^{-k} y_0, \dots, y_0, \dots, A^l y_0 \right).$$

Note, that the residual in this approach is also rank-1 and can be cheaply computed. This approach was implemented as the Krylov plus Inverted Krylov algorithm (hereafter KPIK) in [32] and convergence estimate also was obtained.

The second approach is the Rational Krylov Subspace Method (RKSM) which was proposed in [8]. Its main idea is to compute vectors step by step from the rational Krylov subspaces

$$\text{span} \left((A + s_i I)^{-1} y_0, \quad i = 1, \dots \right).$$

The shifts s_i are selected by a special procedure. There are different algorithms to compute the shifts (and the method proposed in this paper falls into this class, also

there is a recent algorithm [10] based on tangential interpolation). We use the RKSM method described in [9] which has the publicly available implementation. The MATLAB code of both methods can be downloaded from <http://www.dm.unibo.it/~simoncin/software.html>. ■

Note that it is not fully fair to compare the efficiency of the ALR and KPIK with RKSM. The first two methods use vectors from Krylov subspace and have $2r + 1$ size of approximation subspaces at r iteration step, in but “pure” RKSM method has a basis of size $(r + 1)$ after r iterations. We tried to “extend” the RKSM method by adding Krylov vectors. This extended approach we will call *ERKSM*.

4.1. Efficient implementation. Note that the KPIK method has important feature. It uses only linear solver with the matrix A at every step of algorithm, so the factorization of the matrix A can significantly reduce the complexity. Another methods (ALR, RKSM, ERKSM) solve linear systems with different matrices so this method is not applicable. Instead, we propose to use the algebraic multigrid to speed-up the solution of linear systems and to use the same multigrid hierarchy for different shifted systems. Algebraic multigrid (AMG) is a method for the solution of linear systems based on the multigrid principles, but requires no explicit knowledge of the problem geometry. AMG determines coarse grids, intergrid transfer operators, and coarse-grid equations based solely on the matrix entries. Denote vector spaces \mathbf{R}^n and \mathbf{R}^{n_c} that correspond to the fine and the coarse grids. Interpolation (prolongation) maps the coarse grid to the fine grid and is represented by the $n \times n_c$ matrix $P_c : \mathbf{R}^{n_c} \rightarrow \mathbf{R}^n$. There are also few options for defining the coarse system A_c and the most common approach is to use the Galerkin projection $A_c = P_c^T A P_c$. Our main idea is to use the algebraic multigrid method with the Galerkin projection to construct the fast solver for “shifted” linear systems with matrices $(A + sI_n)$. Note that if the transfer operators are chosen to be the same for all shifts s , then the coarse system matrix can be easy “shifted” $A_c + I_{n_c} = P_c^T (A + sI_n) P_c$. We use the Python implementation of AMG [3] to find the coarse grid hierarchy for the matrix A once and then reuse this hierarchy for shifted linear systems. This trick is possible because the matrix A is stable and the shifts always have negative real parts. We found that these approach works well both in symmetric and non-symmetric cases in our numerical experiments.

We have chosen 9 methods for the comparison. First 4 methods are ALR, KPIK, RKSM and ERKSM with shifted linear systems solved using direct solvers for sparse matrices. The next 4 methods use the modified AMG solver. And the last method is KPIK with factorized inverse, and we denote it KPIK(LU).

4.2. Model problem 1: Laplace2D matrix. We start our tests on symmetric problems. The first problem is the discretization of the two-dimensional Laplace operator

$$Lu = u_{xx} + u_{yy}$$

with Dirichlet boundary conditions on the unit square using 5-point stencil operator. The vector y_0 is obtained by the discretization on the grid of the function

$$f(x, y) = e^{-(x-0.5)^2 - 1.5(y-0.7)^2}.$$

The results are shown in Table 4.1, final time shows the computational time in which the method reaches 10^{-8} accuracy.

Table 4.1: Model problem 1 timings

grid	method	precomp.	1 solver time	final time	it-s/rank
64×64	ALR	–	0.0190	0.2303	10/21
	ALR(AMG)	0.0695	0.0498	0.5703	10/21
	KPIK(LU)	0.0341	0.0018	0.1755	15/31
	KPIK(AMG)	0.0695	0.0319	0.6104	15/31
	KPIK	–	0.0196	0.3654	15/31
	RKSM	0.1345	0.0194	1.8460	21/22
	RKSM(AMG)	0.2040	0.0434	2.4254	21/22
	ERKSM	0.1345	0.0210	2.7598	18/37
	ERKSM(AMG)	0.2040	0.0533	3.4273	18/37
128×128	ALR	–	0.0981	1.3168	12/25
	ALR(AMG)	0.1941	0.1431	2.5503	12/25
	KPIK(LU)	0.1746	0.0066	1.0401	20/41
	KPIK(AMG)	0.1941	0.1018	2.9015	20/41
	KPIK	–	0.1051	2.7162	20/41
	RKSM	1.0598	0.1024	5.1593	22/23
	RKSM(AMG)	1.2539	0.1751	7.4457	23/24
	ERKSM	1.0598	0.1063	9.2354	25/51
	ERKSM(AMG)	1.2539	0.1819	10.5334	23/47
256×256	ALR	–	0.6541	10.7695	15/31
	ALR(AMG)	0.6764	0.6083	13.1072	15/31
	KPIK(LU)	1.1841	0.0399	9.5395	26/53
	KPIK(AMG)	0.6764	0.4087	17.2390	26/53
	KPIK	–	0.6728	21.4517	26/53
	RKSM	29.7068	0.7498	55.8941	27/28
	RKSM(AMG)	30.3832	0.9082	59.5665	26/27
	ERKSM	29.7068	0.7158	58.3618	24/49
	ERKSM(AMG)	30.3832	1.0387	68.0542	24/49

Note that for the 256×256 grid the RKSM-based methods have significant pre-computation time, in which the eigenvalue bounds are estimated. The KPIK(LU) method is significantly faster than other methods on all grids. Note that the AMG solver is slower than the direct solver as well. Another noticeable feature of the AMG solver is the significant variation of average linear system solution time on the 256×256 grid for different shift selection strategies. The main reason of such variation is that the “shifted” multigrid hierarchy may take more time in case of relatively big shifts. An example of the shift distribution is presented on Figure 4.1.

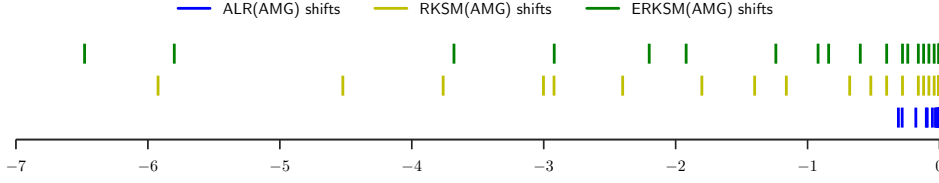


Fig. 4.1: Shift distributions for different methods

4.3. Model problem 2: Laplace3D matrix. The second problem is taken from [32, Example 5.3] and it is the discretization of the three-dimensional Laplace operator

$$Lu = u_{xx} + u_{yy} + u_{zz}$$

with Dirichlet boundary conditions on the unit square using 7-point stencil operator. The vector y_0 was taken to be the vector of all ones. The results are shown in Table 4.2,

4.4. Model problem 3. The third problem is taken from [32, Example 5.1] and describes a model of heat flow with convection in the given domain. The associated differential operator is

$$Lu = u_{xx} + u_{yy} - 10xu_x - 1000yu_y$$

on the unit square with Dirichlet boundary conditions. Matrices A are obtained from the central finite difference discretization of the differential operator using 5-point stencil operator and are non-symmetric with complex eigenvalues. Once again, the vector y_0 was taken to be the vector of all ones. The results are shown in Table 4.3. For this problem KPIK method with LU factorization is the best one on all grids.

4.5. Model problem 4. The fourth problem is taken from [32, Example 5.2] and it is a three-dimensional variant of the previous problem. The differential operator is given by

$$Lu = u_{xx} + u_{yy} + u_{zz} - 10xu_x - 1000yu_y - u_z$$

with Dirichlet boundary conditions on the unit cube using 7-point stencil operator. Once again, the vector y_0 was taken to be the vector of all ones. The results are shown in Table 4.4. The LU-factorization takes too long on the finest grid for 3D problems so KPIK method which uses AMG solver is faster than KPIK(LU) is faster. The ALR(AMG) method is the fastest for the $30 \times 30 \times 30$ grid.

5. Conclusions and future work. The existing methods for the low-rank approximation to the solution of the Lyapunov equations perform quite well on different problems, provided the right implementation of the linear system solver with shifted matrices is available. The ALR method in this paper produces different shifts in comparison with the RKSM solver: the shifts computed by the ALR method are less spread and this gives a possibility to reuse the multigrid hierarchy in a more efficient way, and we think it is the most promising feature of our method (and the number of iterations is similar to the RKSM/ERKSM methods). In our future work we plan to investigate the properties of the proposed approach. First of all, we would like to

Table 4.2: Model problem 2 timings

grid	method	precomp.	1 solver time	final time	it-s/rank
10×10×10	ALR	–	0.0147	0.0822	5/11
	ALR(AMG)	0.0712	0.0113	0.1286	5/11
	KPIK(LU)	0.0163	0.0006	0.0303	6/13
	KPIK(AMG)	0.0712	0.0136	0.1521	6/13
	KPIK	–	0.0116	0.0684	6/13
	RKSM	0.0054	0.0102	0.3186	9/10
	RKSM(AMG)	0.0766	0.0099	0.3205	9/10
	ERKSM	0.0054	0.0142	0.3081	6/13
	ERKSM(AMG)	0.0766	0.0146	0.3729	6/13
20×20×20	ALR	–	0.6237	3.8685	7/15
	ALR(AMG)	0.1385	0.0993	0.7724	7/15
	KPIK(LU)	0.8283	0.0085	0.9671	8/17
	KPIK(AMG)	0.1385	0.0766	0.7419	8/17
	KPIK	–	0.6313	4.4834	8/17
	RKSM	0.0608	0.6303	6.0856	10/11
	RKSM(AMG)	0.1993	0.0846	1.3038	10/11
	ERKSM	0.0608	0.6811	6.9582	10/21
	ERKSM(AMG)	0.1993	0.0832	1.5275	9/19
30×30×30	ALR	–	8.9842	62.6705	8/17
	ALR(AMG)	0.4265	0.3449	3.0680	8/17
	KPIK(LU)	19.0281	0.0535	19.9242	10/21
	KPIK(AMG)	0.4265	0.2354	2.9497	10/21
	KPIK	–	9.1710	82.3441	10/21
	RKSM	0.3609	9.0977	120.1328	14/15
	RKSM(AMG)	0.7874	0.3443	6.2245	14/15
	ERKSM	0.3609	10.2733	115.8494	12/25
	ERKSM(AMG)	0.7874	0.3836	6.5964	11/23

prove the convergence of the method. It will be also very interesting to generalize it to the rank- r right-hand side, and also to extend it to other matrix functions. The effect of inexact solvers on the convergence of the ALR method also need to be studied.

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REFERENCES

- [1] Z. BAI, *Krylov subspace techniques for reduced-order modeling of large-scale dynamical systems*, APPL NUMER MATH, (2002).

Table 4.3: Model problem 3 timings

grid	method	precomp.	1 solver time	final time	it-s/rank
64×64	ALR	–	0.0184	0.1834	8/17
	ALR(AMG)	0.1744	0.0253	0.3649	8/17
	KPIK(LU)	0.0197	0.0017	0.1575	11/23
	KPIK(AMG)	0.1744	0.0284	0.5586	11/23
	KPIK	–	0.0250	0.3809	11/23
	RKSM	0.0452	0.0177	0.7313	12/13
	RKSM(AMG)	0.2196	0.0185	0.7349	12/13
	ERKSM	0.0452	0.0183	0.7154	9/19
	ERKSM(AMG)	0.2196	0.0187	1.0360	10/21
128×128	ALR	–	0.1189	1.2058	10/21
	ALR(AMG)	0.5329	0.0875	1.6560	10/21
	KPIK(LU)	0.1136	0.0098	0.6804	11/23
	KPIK(AMG)	0.5329	0.1052	2.0300	11/23
	KPIK	–	0.1278	1.5739	11/23
	RKSM	0.6967	0.1241	3.0168	13/14
	RKSM(AMG)	1.2296	0.0758	2.7024	13/14
	ERKSM	0.6967	0.1225	3.5379	12/25
	ERKSM(AMG)	1.2296	0.0698	3.2370	11/23
256×256	ALR	–	1.1270	14.2010	10/21
	ALR(AMG)	0.7507	0.3281	5.1982	10/21
	KPIK(LU)	1.0185	0.0313	3.0908	12/25
	KPIK(AMG)	0.7507	0.2982	5.6122	12/25
	KPIK	–	1.4760	18.2555	12/25
	RKSM	6.8556	1.0914	27.0884	17/18
	RKSM(AMG)	7.6063	0.2696	14.1912	17/18
	ERKSM	6.8556	1.1761	29.3055	15/31
	ERKSM(AMG)	7.6063	0.2524	15.1329	13/27

- [2] C. A. BEATTIE AND S. GUGERCIN, *Krylov-based minimization for optimal \mathcal{H}^2 model reduction*, in 46th IEEE conference on decision and control, 2007, pp. 4385–4390.
- [3] W. N. BELL, L. N. OLSON, AND J. B. SCHRODER, *PyAMG: Algebraic multigrid solvers in Python v2.0*, 2011. Release 2.0.
- [4] P. BENNER, P. KÜRSCHNER, AND J. SAAK, *Self-generating and efficient shift parameters in ADI methods for large Lyapunov and Sylvester equations*, GAMM-Mitteilungen, 17 (2013), pp. 123–143.
- [5] P. BENNER, J.-R. LI, AND T. PENZL, *Numerical solution of large-scale Lyapunov equations, Riccati equations, and linear-quadratic optimal control problems*, Numer. Linear Algebr., 15 (2008), pp. 755–777.
- [6] T. DAMM, *Direct methods and adi-preconditioned Krylov subspace methods for generalized Lyapunov equations*, Numer. Linear Algebr., 15 (2008), pp. 853–871.
- [7] V. DRUSKIN AND L. KNIZHNERMAN, *Extended Krylov subspaces: approximation of the matrix square root and related functions*, SIAM J Matrix Anal A, 19 (1998), pp. 755–771.
- [8] V. DRUSKIN, C. LIEBERMAN, AND M. ZASLAVSKY, *On adaptive choice of shifts in rational Krylov subspace reduction of evolutionary problems*, SIAM J. Sci. Comput., 32 (2010), pp. 2485–2496.
- [9] V. DRUSKIN AND V. SIMONCINI, *Adaptive rational Krylov subspaces for large-scale dynamical*

Table 4.4: Model problem 4 timings

grid	method	precomp.	1 solver time	final time	it-s/rank
10×10×10	ALR	–	0.0117	0.0671	5/11
	ALR(AMG)	0.0444	0.0066	0.0952	5/11
	KPIK(LU)	0.0181	0.0004	0.0386	7/15
	KPIK(AMG)	0.0444	0.0099	0.1206	7/15
	KPIK	–	0.0257	0.1760	7/15
	RKSM	0.0041	0.0108	0.2189	7/8
	RKSM(AMG)	0.0485	0.0094	0.2259	7/8
	ERKSM	0.0041	0.0128	0.2201	5/11
	ERKSM(AMG)	0.0485	0.0085	0.2276	5/11
20×20×20	ALR	–	0.6424	3.2881	6/13
	ALR(AMG)	0.2231	0.0466	0.5020	6/13
	KPIK(LU)	0.6687	0.0086	0.8351	9/19
	KPIK(AMG)	0.2231	0.0436	0.6787	9/19
	KPIK	–	0.8533	7.0838	9/19
	RKSM	0.0265	0.6610	5.5919	9/10
	RKSM(AMG)	0.2496	0.0491	0.9061	9/10
	ERKSM	0.0265	0.7303	4.8876	7/15
	ERKSM(AMG)	0.2496	0.0541	0.9108	6/13
30×30×30	ALR	–	9.2135	53.2061	7/15
	ALR(AMG)	0.9827	0.1987	2.3924	7/15
	KPIK(LU)	10.1743	0.0497	11.0392	9/19
	KPIK(AMG)	0.9827	0.2055	3.0282	9/19
	KPIK	–	12.7750	105.1641	9/19
	RKSM	0.1215	9.3640	85.8903	10/11
	RKSM(AMG)	1.1042	0.1792	3.2822	10/11
	ERKSM	0.1215	9.5372	58.2637	7/15
	ERKSM(AMG)	1.1042	0.1609	3.2703	8/17

systems, Systems & Control Letters, 60 (2011), pp. 546–560.

- [10] V. DRUSKIN, V. SIMONCINI, AND M. ZASLAVSKY, *Adaptive tangential interpolation in rational Krylov subspaces for MIMO dynamical systems*, SIAM J Matrix Anal A, 35 (2014), pp. 476–498.
- [11] G. FLAGG, C. BEATTIE, AND S. GUGERCIN, *Convergence of the iterative rational Krylov algorithm*, Syst. Control. Lett., 61 (2012), pp. 688–691.
- [12] S. GUGERCIN, *An iterative rational Krylov algorithm (IRKA) for optimal \mathcal{H}^2 model reduction*, in Householder Symposium XVI, Seven Springs Mountain Resort, PA, USA, 2005.
- [13] S. GUGERCIN, A. C. ANTOLAS, AND C. BEATTIE, *\mathcal{H}^2 model reduction for large-scale linear dynamical systems*, SIAM J. Matrix Anal. A., 30 (2008), pp. 609–638.
- [14] S. GUGERCIN, D. C. SORESENSEN, AND A. C. ANTOLAS, *A modified low-rank Smith method for large-scale Lyapunov equations*, Numer Algorithms, 32 (2003), pp. 27–55.
- [15] T. HINAMOTO, *2-d Lyapunov equation and filter design based on the Fornasini-Marchesini second model*, IEEE Trans. Circuits Syst. I, Fundam. Theory Appl., 40 (1993), pp. 102–110.
- [16] M. HOCHBRUCK AND G. STARKE, *Preconditioned Krylov subspace methods for Lyapunov matrix equations*, SIAM J. Matrix Anal. Appl., 16 (1995), pp. 156–171.
- [17] I. M. JAIMOUKHA AND E. M. KASENALLY, *Krylov subspace methods for solving large Lyapunov*

- equations*, SIAM J. Numer. Anal., 31 (1994), pp. 227–251.
- [18] K. JBILOU, *ADI preconditioned Krylov methods for large Lyapunov matrix equations*, Linear Algebra Appl., 432 (2010), pp. 2473–2485.
 - [19] K. JBILOU AND A. RIQUET, *Projection methods for large Lyapunov matrix equations*, Linear Algebra Appl., 415 (2006), pp. 344–358.
 - [20] A. J. LAUB, *A schur method for solving algebraic Riccati equations*, IEEE Trans. Autom. Control, 24 (1979), pp. 913–921.
 - [21] V. I. LEBEDEV, *On a Zolotarev problem in the method of alternating directions*, USSR Computational Mathematics and Mathematical Physics, 17 (1977), pp. 58–76.
 - [22] J.-R. LI, F. WANG, AND J. K. WHITE, *An efficient Lyapunov equation-based approach for generating reduced-order models of interconnect*, in Proceedings of the 36th annual ACM/IEEE Design Automation Conference, ACM, 1999, pp. 1–6.
 - [23] J.-R. LI AND J. WHITE, *Low rank solution of Lyapunov equations*, SIAM J. Matrix Anal. and Appl., 24 (2002), pp. 260–280.
 - [24] A. LU AND E. L. WACHSPRESS, *Solution of Lyapunov equations by alternating direction implicit iteration*, Comput. Math. Appl., 21 (1991), pp. 43–58.
 - [25] C. C. K. MIKKELSEN, *Any positive residual curve is possible for the Arnoldi method for Lyapunov matrix equations*, tech. rep., Tech. Rep. UMINF 10.03, Department of Computing Science and HPC2N, UmeåUniversity, 2010.
 - [26] T. PENZL, *A cyclic low-rank Smith method for large sparse Lyapunov equations*, SIAM J. on Sci. Comput., 21 (1999), pp. 1401–1418.
 - [27] J.-B. POMET AND L. PRALY, *Adaptive nonlinear regulation: estimation from the Lyapunov equation*, Automatic Control, IEEE Transactions on, 37 (1992), pp. 729–740.
 - [28] Y. SAAD, *Numerical solution of large Lyapunov equations*, Research Institute for Advanced Computer Science, NASA Ames Research Center, 1989.
 - [29] ———, *Overview of Krylov subspace methods with applications to control problems*, Research Institute for Advanced Computer Science, NASA Ames Research Center, 1989.
 - [30] Y. SAAD, *Iterative methods for sparse linear systems*, 2003.
 - [31] J. M. SANCHES, J. C. NASCIMENTO, AND J. S. MARQUES, *Medical image noise reduction using the Sylvester–Lyapunov equation*, IEEE Trans. Image Process., 17 (2008), pp. 1522–1539.
 - [32] V. SIMONCINI, *A new iterative method for solving large-scale Lyapunov matrix equations*, SIAM J. Sci. Comput., 29 (2007), pp. 1268–1288.
 - [33] V. SIMONCINI, *Computational methods for linear matrix equations*, tech. rep., 2013.
 - [34] V. SIMONCINI AND V. DRUSKIN, *Convergence analysis of projection methods for the numerical solution of large Lyapunov equations*, SIAM J. Numer. Anal., 47 (2009), pp. 828–843.
 - [35] D. SORESENSEN AND A. ANTOUNAS, *The Sylvester equation and approximate balanced reduction*, LINEAR ALGEBRA APPL, 351 (2002), pp. 671–700.
 - [36] T. STYKEL AND V. SIMONCINI, *Krylov subspace methods for projected Lyapunov equations*, Appl. Numer. Math., 62 (2012), pp. 35–50.
 - [37] B. VANDEREYCKEN, *Riemannian and multilevel optimization for rank-constrained matrix problems*, PhD thesis, PhD thesis, Katholieke Universiteit Leuven, 2010.
 - [38] B. VANDEREYCKEN AND S. VANDEWALLE, *A Riemannian optimization approach for computing low-rank solutions of Lyapunov equations*, SIAM J. Matrix Anal. Appl., 31 (2010), pp. 2553–2579.
 - [39] E. L. WACHSPRESS, *Iterative solution of the Lyapunov matrix equation*, Appl. Math. Lett., 1 (1988), pp. 87–90.